Figure 1. The geometry for a part of an engine exhaust manifold from the Volvo Car corporation is shown at left as a set of "trimmed NURBS" patches read in from an IGES file. Because of errors in the IGES description, some features are incorrectly represented. The image at right shows the geometry after repair with Rapsodi's interactive RAP tool.

Rapsodi

Rapid Problem Setup for Diverse Mesh-based Simulations

Technology

The Rapsodi project performs research and develops algorithms aimed at enhancing the ability to rapidly set up computational geometry for large-scale scientific simulations that are based on the solution of partial differential equations in three space dimensions. Current problem setup technology often requires weeks or months to perform this initial setup step, and even incremental changes in geometry can require complete regeneration of the computational mesh. Rapsodi envisions a scenario wherein a complex problem can be set up in a matter of hours and a simulation run overnight, leaving the scientist ready to reformulate the problem specification the next morning and repeat the process. This research project is overcoming the remaining major technical obstacles by focusing a computational science research effort on the critical issues involved.

Many of the computational simulation projects at Lawrence Livermore National Laboratory (LLNL) involve the solution of partial differential equations (PDEs) in complex 3D geometric configurations. A significant, recognized area of deficiency in our capability to perform these simulations arises from the inability to rapidly set up and easily modify the computational geometries. The problem setup process consists of all the steps needed to take a description produced, for example, using computer-aided design (CAD) and convert it into a 3D volumetric mesh that can be used for simulation and analysis. Currently, using state-of-the-art mesh generation software takes scientists weeks or even months to generate a new computational mesh from scratch. Rapsodi is developing algorithms and tools that will help reduce this setup time to less than a day for a significant fraction of the simulation and analysis applications at LLNL.

Construction of Water-tight Surface Geometry from CAD Data

Because geometry specifications such as CAD were not designed with mesh construction in mind, there are few standard tools for converting them to parameterizations that can readily be used by mesh generation tools. Rapsodi interacts with CAD descriptions through a common file format called Initial Graphics Exchange Specifications (IGES) that is supported by most common CAD packages. The representation extracted from an IGES file is a set of trimmed spline patches (NURBS) that completely cover the surface. This representation is often not "water tight" or single-valued. Converting the input geometry to a representation appropriate for simulation and analysis can therefore include repairing the CAD by filling gaps, reconciling errors in NURBS trimming curves, determining NURBS surface connectivity information, and removing unnecessary engineering details from the specification. The RAP software tool, available from the Center for Applied Scientific Computing (CASC) at LLNL, allows much of this work to be done very quickly through an interactive graphics user interface.

Overset or Mixed-Element Mesh Generation

Once the CAD geometry has been cleaned up and repaired, it can be used for simulation and analysis. One possibility is to use it to generate an overset or mixed-element computational mesh. Information from the NURBS representation is used to subdivide the surface representation into components that are then individually meshed. As a practical matter, the component meshes must be generated within seconds on a typical scientific workstation; this necessitates the development of very fast algorithms for evaluating the NURBS representation. Rapsodi software automatically determines adjacency information and constructs a reference triangularization of the surface. Evaluating a point on the geometry surface can then be done much more rapidly by first locating its reference triangle and then using this to find the original location on the patched NURBS surface.

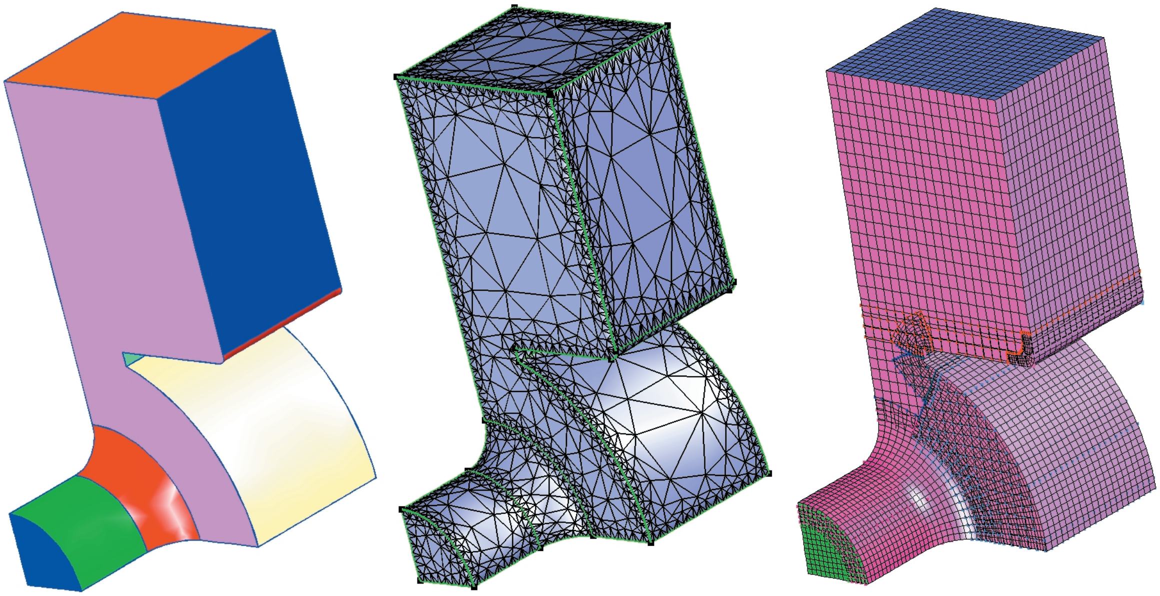

Figure 2. Two steps in the construction of a mesh from a repaired CAD description are shown here. The cleaned up surface geometry is shown at the left. In the middle is a reference triangulation, constructed on each of the patches in the NURBS description of this high-energy accelerator waveguide cavity. This step also determines the connectivity of the patches and reconciles overlaps and gaps between adjacent patches. The reference triangulation is used to accelerate the construction of the overlapping volume mesh shown at right.

A set of surface meshes is then constructed that covers the computational geometry. This is done using a marching technique called "hyperbolic grid generation" in which a partial differential equation is solved for the coordinates of the surface mesh. From the surface meshes, volume "component meshes" are built. The overall hybrid mesh is then constructed by connecting the component meshes with regions of high-quality unstructured mesh using an advancing front technique. This results in an unstructured mesh over which the user has considerable control, and which has large regions of structure that can be exploited for accuracy and efficiency in the ultimate application code.

Embedded Boundary Mesh Generation

The cleaned up and repaired geometry from RAP can also be used to generate other types of computational meshes. An embedded boundary mesh is a Cartesian mesh in two or three dimensions in which complex boundaries are represented as a surface cutting through the mesh. In order to solve partial differential equations on such a mesh, a regular Cartesian mesh method is used everywhere except in the mesh cells that are cut by the boundary, in which special formulas are used to approximate the differential equation and the effect of the boundary conditions. In collaboration with the SciDAC APDEC Center, we have developed a capability based on RAP and the Cartesian 3D mesh generation package CART3D from NASA that allows us to rapidly build embedded boundary meshes either from CAD descriptions or through the use of the elementary geometry building tools available within RAP. A highly resolved water-tight surface triangulation is constructed from the CAD description and used to cut cells in the Cartesian mesh.

Rapsodi is partially funded by the SciDAC program in the DOE Office of Advanced Scientific Computing Research.

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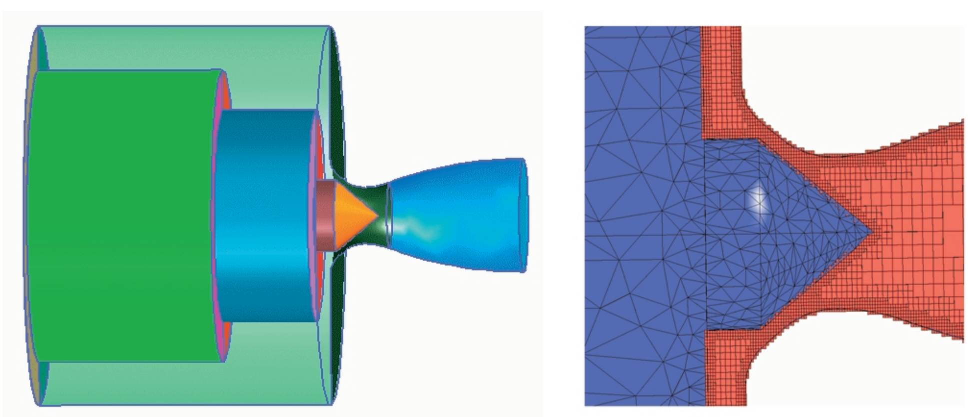

Figure 3. Original geometry (left) and embedded boundary mesh detail (right) for a gas injection nozzle prototype for a plasma-based electron accelerator experiment at Lawrence Berkeley National Laboratory. The surface triangulation is shown on the poppet in blue. One cut plane of the locally refined embedded boundary mesh inside the nozzle region is shown in red.

This work was performed under the auspices of the U.S. Department of Energy by University of California Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.